

WHAT IS CLAIMED IS:

1. A nuclear magnetic resonance method for identifying a site in a DNA-binding and dimerization domain of a papillomavirus E2 protein, the method comprising:

providing a first set of chemical shifts for atoms of a mixture comprising a ligand and the papillomavirus E2 protein;

comparing the first set of chemical shifts to a second set of chemical shifts as listed in Table 1; and

identifying at least a portion of the atoms that exhibit changes in chemical shifts, wherein the site comprises the identified atoms.

2. The method of claim 1 wherein providing the first set of chemical shifts comprises:

providing a mixture of the ligand and the papillomavirus E2 protein;

allowing the ligand to interact with the papillomavirus E2 protein;

obtaining a nuclear magnetic resonance spectrum of the mixture; and

measuring chemical shifts of atoms from the spectrum.

3. The method of claim 2 wherein allowing the ligand to interact comprises allowing the ligand and the protein to reach a binding equilibrium.

4. The method of claim 1 wherein the site is a ligand binding site.

5. The method of claim 1 wherein the papillomavirus E2 protein is encoded by the HPV-18 strain.

6. The method of claim 1 wherein identifying at least a portion of the atoms comprises identifying at least one proton that either exhibits a change in ^1H chemical shift of at least about 0.04 ppm or is no longer observed.

7. The method of claim 1 wherein identifying at least a portion of the atoms comprises identifying at least one carbon atom that either exhibits a change in ^{13}C chemical shift of at least about 0.2 ppm or is no longer observed.
8. The method of claim 1 wherein identifying at least a portion of the atoms comprises identifying at least one nitrogen atom that either exhibits a change in ^{15}N chemical shift of at least about 0.2 ppm or is no longer observed.
9. A nuclear magnetic resonance method for identifying a site in a DNA-binding and dimerization domain of a papillomavirus E2 protein, the method comprising:
 - providing a first ^1H - ^{15}N heteronuclear single quantum correlation spectrum of a mixture comprising a ligand and the papillomavirus E2 protein;
 - comparing the first ^1H - ^{15}N heteronuclear single quantum correlation spectrum to a second ^1H - ^{15}N heteronuclear single quantum correlation spectrum as illustrated in Figure 2; and
 - identifying at least a portion of the amino acids having atoms that exhibit changes in chemical shifts, wherein the site comprises the identified amino acids.
10. The method of claim 9 wherein providing the first spectrum comprises:
 - providing a mixture of the ligand and the papillomavirus E2 protein;
 - allowing the ligand to interact with the papillomavirus E2 protein; and
 - obtaining a ^1H - ^{15}N heteronuclear single quantum correlation spectrum of the mixture.
11. The method of claim 10 wherein allowing the ligand to interact comprises allowing the ligand and the protein to reach a binding equilibrium.
12. The method of claim 9 wherein the site is a ligand binding site.

13. The method of claim 9 wherein the papillomavirus E2 protein is encoded by the HPV-18 strain.
14. The method of claim 9 wherein identifying at least a portion of the amino acids comprises identifying at least one amino acid having a proton that either exhibits a change in ¹H chemical shift of at least about 0.04 ppm or is no longer observed.
15. The method of claim 9 wherein identifying at least a portion of the amino acids comprises identifying at least one amino acid having a nitrogen atom that either exhibits a change in ¹⁵N chemical shift of at least about 0.2 ppm or is no longer observed.
16. A machine-readable data storage medium comprising a data storage material encoded with nuclear magnetic resonance chemical shifts as listed in Table 1, wherein when a first set of chemical shifts is provided, the chemical shifts encoded on the data storage material are capable of being read by the machine to create a second set of chemical shifts, and the machine having programmed instructions that are capable of causing the machine to compare the first and second sets of chemical shifts to arrive at structural information.
17. A computer-assisted method for identifying a ligand binding site in a DNA-binding and dimerization domain of a papillomavirus E2 protein, the method comprising:
providing a first set of nuclear magnetic resonance chemical shifts for atoms of a mixture comprising the ligand and the papillomavirus E2 protein;
causing the first set of chemical shifts to be entered into memory of a computer;

causing the computer to read a second set of chemical shifts as listed in Table 1 from a machine-readable data storage medium;
causing the computer to compare the first and second sets of chemical shifts; and
causing the computer to identify at least a portion of the atoms that exhibit changes in chemical shifts, wherein the ligand binding site comprises the identified atoms.

18. The method of claim 17 wherein the papillomavirus E2 protein is encoded by the HPV-18 strain.
19. The method of claim 17 wherein causing the computer to identify at least a portion of the atoms comprises causing the computer to identify at least one proton that either exhibits a change in ^1H chemical shift of at least about 0.04 ppm or is no longer observed.
20. The method of claim 17 wherein causing the computer to identify at least a portion of the atoms comprises causing the computer to identify at least one carbon atom that either exhibits a change in ^{13}C chemical shift of at least about 0.2 ppm or is no longer observed.
21. The method of claim 17 wherein causing the computer to identify at least a portion of the atoms comprises causing the computer to identify a nitrogen atom that either exhibits a change in ^{15}N chemical shift of at least about 0.2 ppm or is no longer observed.
22. The method of claim 17 further comprising causing the computer to visually display a spatial arrangement of atoms of the ligand binding site.